
Article

Numerical Simulation of Diffusion in Cylindrical Pores: The Influence of Pore Radius on Particle Capture Kinetics

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Abstract

The diffusion and trapping of particles in complex porous media are fundamental processes in materials science and bioengineering. This study systematically investigates the influence of pore radius on particle capture kinetics within a three-dimensional cylindrical pore containing randomly distributed absorbing traps. Numerical simulations were performed for a wide range of pore radii (from $3a$ to $81a$, a is a minimal length of the problem, arbitrary unit) and trap concentrations M (from 100 to 5,090, these numbers are determined by the pore geometry) using a random walk algorithm. The particle lifetime (τ), characterizing the capture rate, was calculated and analyzed. Results reveal three distinct capture regimes dependent on trap concentration: a diffusion-limited regime at low concentration M ($< 1,000$), a transition regime at medium M ($1,000 < M < 2,000$), and a trap-density-dominated saturation regime at high M ($> 2,000$). For each regime, optimal approximating functions for $\tau(M)$ were identified. Furthermore, empirical relationships between the approximating coefficients and the pore radius were derived, which enable the prediction of particle lifetimes. The findings demonstrate that while the pore radius significantly impacts capture kinetics at low trap densities, its influence diminishes as trap concentration increases, converging towards a universal behavior dominated by trap density.

Keywords: diffusion; capture on traps; porous materials; numerical simulation

1. Introduction

The foundational theory of random walks on lattices with traps was established in [1-4], while the diffusion-reaction kinetics among traps was further developed in [5, 6]. Interest is also driven by the expected new features in particle transport, and its applications [7-11]. A particularly relevant application involves investigating diffusion and trapping processes of active particles within porous dielectric low- k materials [12-15]. This problem is relevant for stability, mechanical strength and process compatibility of low k materials [16].

Additionally, the problem of diffusion in complex heterogeneous media and trapping also appeared in emerging bioengineering fields, e.g., in bone nanostructure [17, 18], cartilage [19], or brain extracellular space [20]. This problem is studied by different methods, including numerical simulation [21, 22, 23].

Furthermore, the process of diffusion in pores has a directed form and this driven transport is called active and it is described in some experimentally important situations. This process was recently considered in detail in [24] and [25, 26].

Recently the theory of the capture on traps in the electric field was developed [27] and the numerical simulation of influence of the electric field in two-dimensional homogeneous media was

performed [28]. However, these results are not included in this paper, because the driven transport in porous media requires a separate study.

In our previous study [29], we reported numerical simulations of particle diffusion in a three-dimensional cylindrical pore with traps for some values of radius of pore $R = 3a, 9a, 27a$, and $81a$, where a denotes the characteristic system length scale. Notably, the behavior observed for $R = 3a, 9a$, and $27a$ differed significantly from that for $R = 81a$.

In this article, we study particle capture in cylindrical pores to account for the influence of pore radius on particle capture kinetics in a wide range of radius such as $R=3a, 6a, 9a, 15a, 18a, 21a, 27a, 30a, 40a, 50a, 60a, 70a, 81a$ in more details. Through comprehensive numerical experiments spanning a broad range of pore radii, we systematically investigate the influence of pore radius on particle capture kinetics by analyzing particle lifetime statistics, developing mathematical approximations for these lifetimes, and characterizing the behavior of the corresponding approximating functions as a function of pore radius.

2. Problem Statement and Simulation Algorithm

We numerically investigate the diffusion of active particles within a cylindrical pore of radius R and height H as a simplified model of porous media. The inner pore surface contains randomly distributed absorbing traps, with the trap concentration varied systematically. The initial condition corresponds to a uniform density of N_0 particles released at the pore entrance (the $Z=0$ plane), simulating a constant particle flux. This setup is motivated by applications such as the diffusion of active species (e.g., oxygen, termed O-particles) through porous materials containing trapping sites (C-particles) [30, 31]. While prior studies have employed one-dimensional approximations with multiple particle types [32, 33], this work focuses explicitly on the influence of the pore radius R on the particle capture kinetics in a three-dimensional geometry.

In this paper, we use the same algorithms as in our previous work [29], which include two main components: the Algorithm for Simulations of Diffusion Processes in Media with Traps and the Algorithm for Placing Traps. We described these algorithms in appendix A and B.

3. Modeling Process and Results of Numerical Simulation

3.1. Particle Lifetime and the Three Capture Regimes

To characterize the rate of particle capture by traps, we define the lifetime parameter, denoted as τ , based on the exponential decay model:

$$N_t = N_0 \exp\left(-\frac{t}{\tau}\right) \quad (1)$$

Here, N_0 is the initial number of particles, and N_t is the number of active particles at iteration t . The lifetime τ corresponds to the characteristic time (in iteration steps) at which the number of particles decreases by a factor of e . Equation (1) describes the simple process of capture on traps with “death” of particle after capture, and the trap can capture particle only one time. However, it differs from CTRW transport [1]. In the CTRW the particles only

delays on the traps and there is a possibility to leave the traps, usually described by delay function with the power law kernel.

Numerical experiments revealed that this exponential dependence stabilizes for pores with radii $3a$, $9a$, and $27a$ when the number of traps satisfies $M \geq 180$ [29]. In contrast, for the larger pore radius $81a$, stabilization requires a higher number of traps ($M \geq 220$). Qualitatively, this behavior arises due to the increased diffusion volume and the consequently reduced probability of particles reaching the pore surface where traps are located.

In this study, we investigated cylindrical pores with radii $R \in \{3a, 6a, 9a, 15a, 18a, 21a, 27a, 30a, 40a, 50a, 60a, 70a, 81a\}$, where a denotes the characteristic length scale of the system. The computed lifetime values τ for each pore radius, derived from numerical simulations under consistent trap concentration and distribution conditions, are comprehensively tabulated in Appendix B.

In diffusion processes within media containing traps, a characteristic length scale emerges—the mean distance between traps—which introduces an associated with diffusion the timescale. For one-dimensional diffusion, this timescale is proportional to the square of the inter-trap distance. In higher dimensions, geometric constraints and pore curvature further influence the capture kinetics, necessitating the systematic analysis presented in this work. For one-dimensional diffusion the characteristic time is equal to:

$$t_c = \frac{1}{Dc^2} \quad (2)$$

In this context, D represents the diffusion coefficient, and c denotes the concentration of traps.

To investigate the influence of pore radius on particle capture kinetics, we analyzed the asymptotic behavior of the lifetime (2) for pores with radii $3a$, $15a$, $18a$, and $21a$. We determine the dependence of the average lifetime $\langle \tau \rangle$ on the number of traps M .

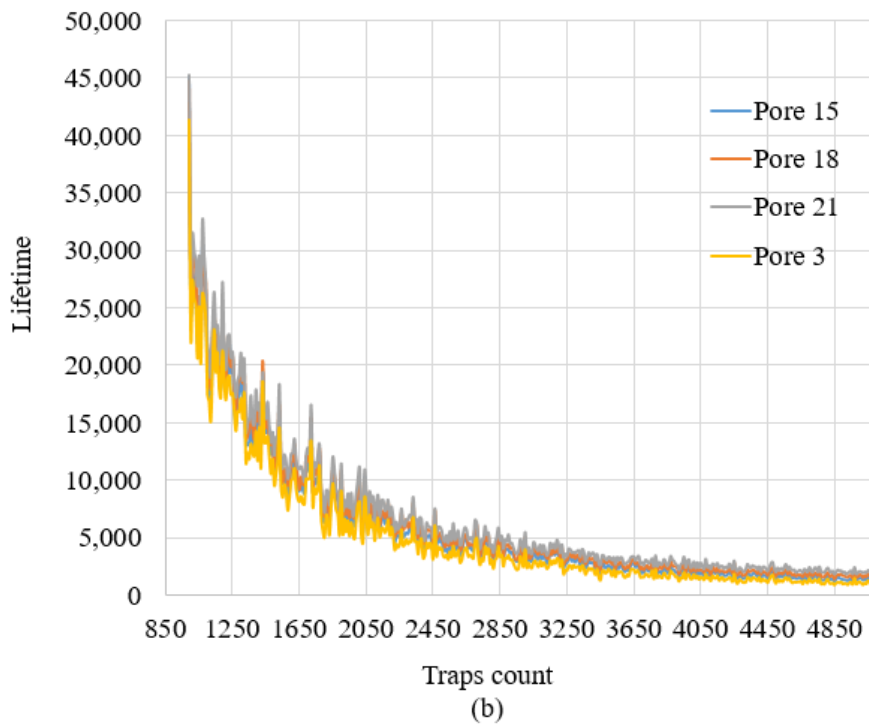
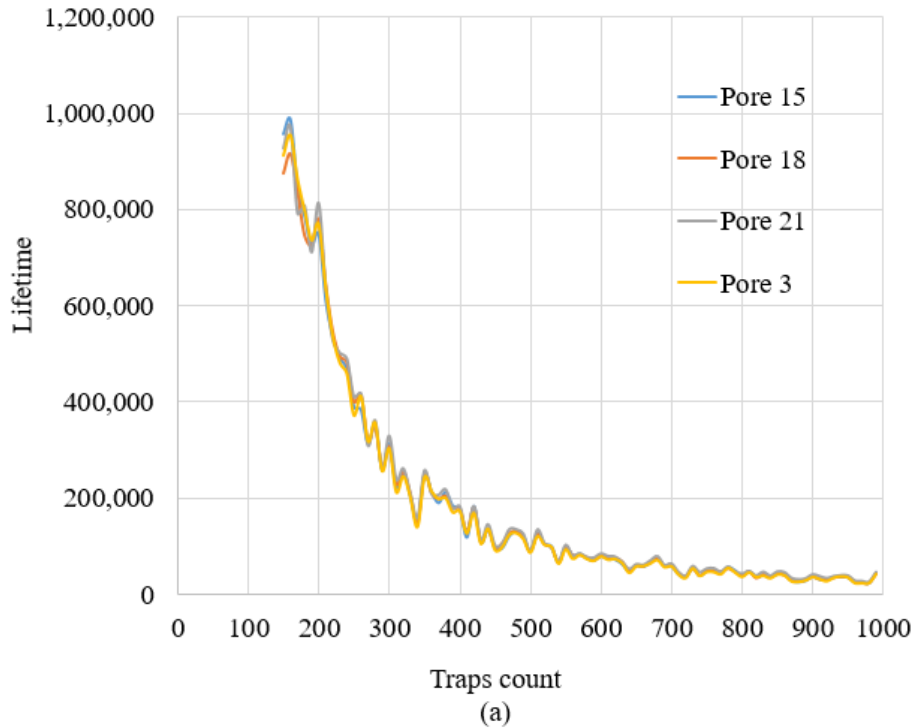


Figure 1. Dependence of particle lifetime (τ) on the number of traps (M) for different pore radii. The top figure (a) corresponds to the low trap concentration regime ($M < 1,000$), while the bottom figure (b) shows the high concentration regime ($M > 1,000$). Figures illustrate the transition from a steep, radius-dependent decrease in lifetime at low M to a convergence towards a plateau at high M , highlighting the diminishing influence of pore geometry with increasing trap density.

The relationship between $\langle \tau \rangle$ and M , illustrated in Fig. 1, exhibits two different regimes:

1. Low trap concentration regime ($M < 1000$): The lifetime $\langle \tau \rangle$ decreases rapidly with increasing M , consistent with the

scaling according to (2). This behavior reflects a diffusion capture process where the mean distance between traps governs the timescale of particle trapping.

2. Trap-density-dominated saturation regime ($M > 1000$):

The lifetime reaches a plateau, indicating that the capture process becomes less sensitive to further increases in trap concentration. In this regime, the system transitions to a state where capture kinetics are dominated by other factors, such as spatial coverage of traps or geometric constraints, rather than by diffusion alone.

These results highlight the critical role of trap concentration and pore radius in determining capture efficiency and provide insight into the underlying mechanisms governing particle trapping in confined geometries.

We analyze the dependence of particle lifetime τ on trap concentration M over the extended range $M \in [1,000; 5,090]$, as shown in Figure 2.

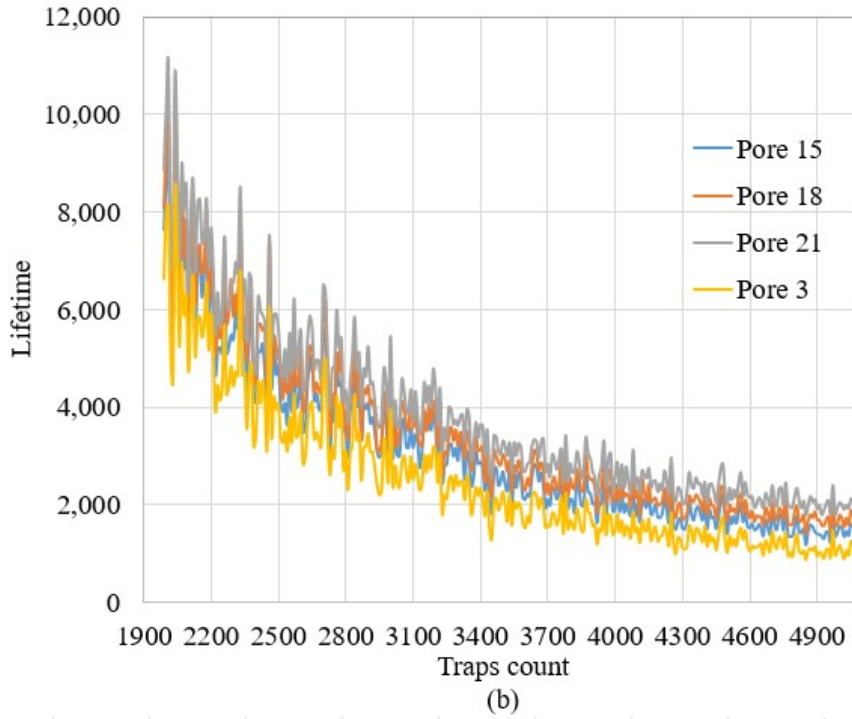
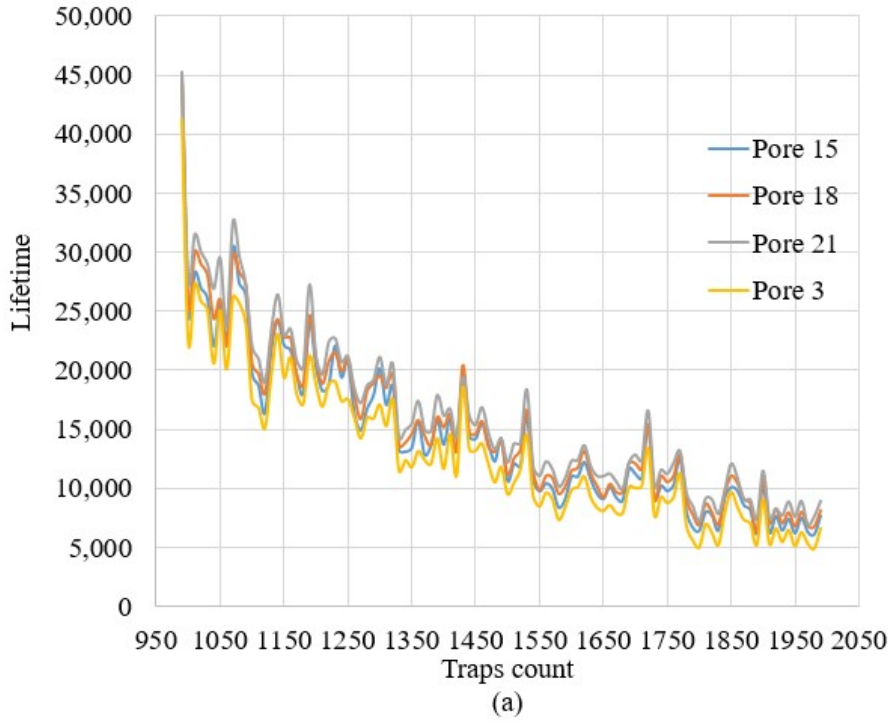


Figure 2. Dependence of particle lifetime (τ) on trap concentration (M) for different pore radii. The top figure (a) displays the medium concentration regime ($1,000 < M < 2,000$), while the bottom figure (b) shows the high concentration regime ($M > 2,000$). The plots demonstrate the continuing convergence of lifetime values across different pore radii with increasing M , indicating the transition to a trap-density-dominated capture process where geometric parameters become less significant.

Analysis of the curves reveals that the qualitative influence of trap concentration on lifetime remains consistent across all pore radii. Specifically,

τ decreases monotonically with increasing M , reflecting enhanced capture efficiency due to higher trap density.

To elucidate the influence of pore radius on particle capture kinetics, we examine in detail the lifetime dynamics within small-radius pores. Figure 3 presents the dependence of the lifetime τ on the number of traps M for pore radii $3a$, $6a$, and $9a$. The behavior of τ for these small radii is nearly identical, suggesting that geometric effects are minimal in this regime.

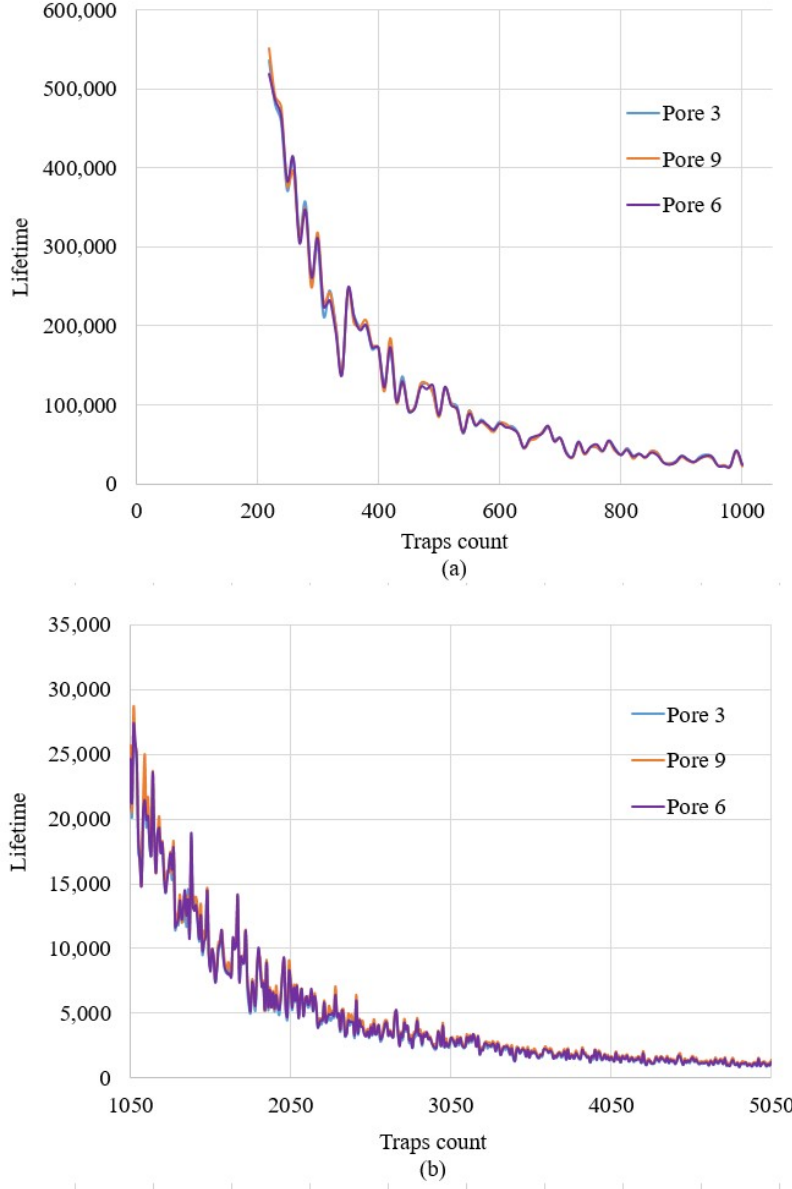


Figure 3. Dependence of particle lifetime (τ) on trap concentration (M) for small-radius pores ($3a$, $6a$, $9a$). The top figure (a) shows the low concentration regime ($M < 1,000$), while the bottom figure (b) presents the high concentration regime ($M > 1,000$).

The nearly identical behavior of the curves for different radii in both regimes demonstrates the unified capture kinetics in small pores, where geometric differences have minimal effect on the diffusion-limited trapping process.

For quantitative analysis, we compute the lifetime difference $\Delta\tau = \tau(3a) - \tau(9a)$ to compare capture efficiency between pores of radii $3a$ and $9a$. Figure 4 illustrates the dependence of $\Delta\tau$ on M . Positive values of $\Delta\tau$ (above the abscissa) indicate a longer lifetime in the $3a$ pore, implying slower capture,

while negative values reflect a longer lifetime in the 9a pore. The observed variation in $\Delta\tau$ with M highlights subtle differences in capture kinetics due to pore size, even when radii are relatively small.

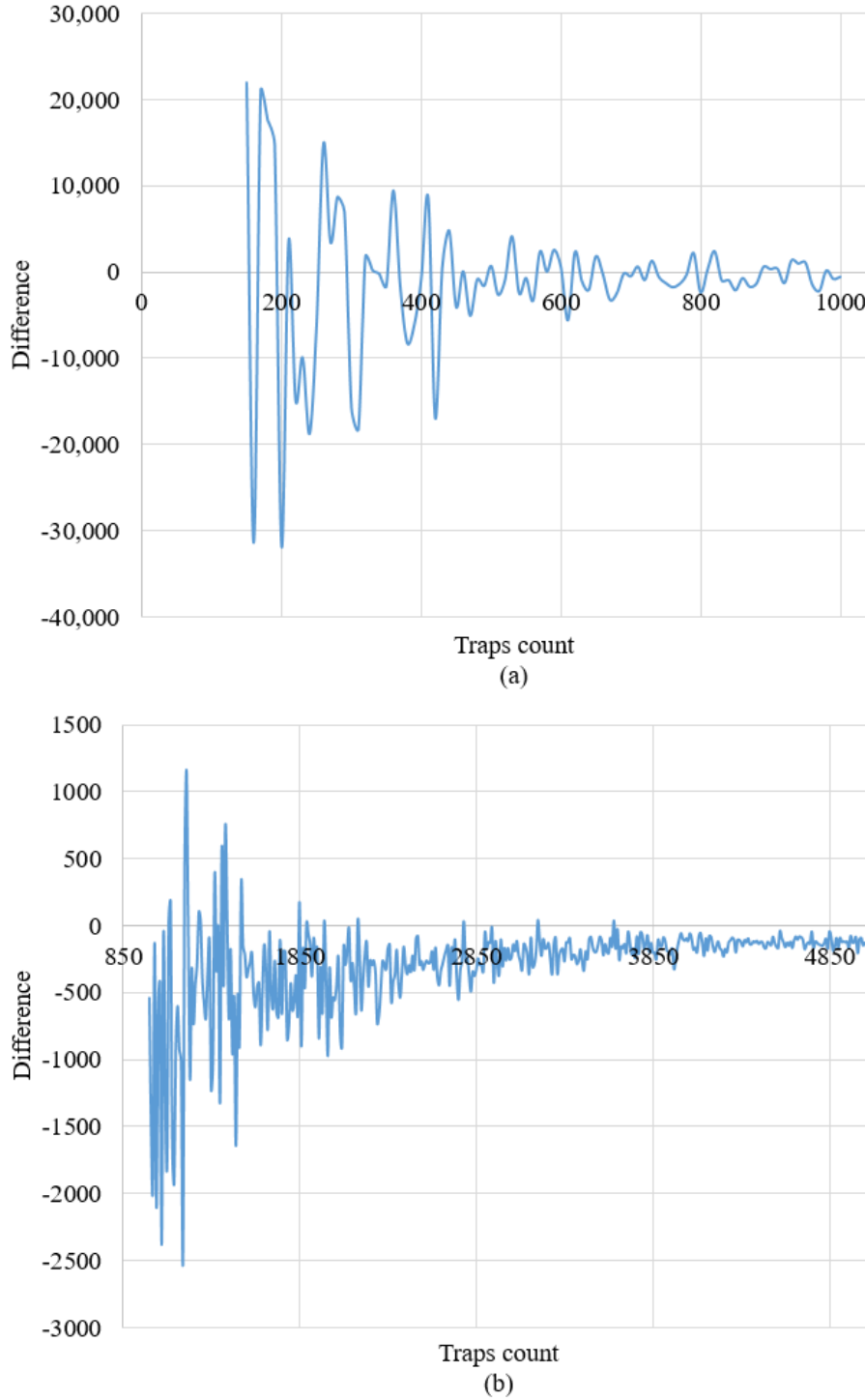


Figure 4. Difference in particle lifetime ($\Delta\tau = \tau_{3a} - \tau_{9a}$) between pores of radii 3a and 9a as a function of trap concentration (M). The top (a) shows the low concentration regime ($M < 1000$), where significant differences in lifetime are observed due to geometric effects. The bottom (b) displays the high concentration regime ($M > 1,000$), demonstrating the convergence of lifetime values as trap density becomes the dominant factor in capture kinetics. Positive $\Delta\tau$ values indicate longer lifetime in the 3a pore.

The dependence of the lifetime difference $\Delta\tau = \tau(3a) - \tau(9a)$ on the number of traps M (Fig. 4) exhibits a monotonic decrease as M increases. The

maximum absolute values of $\Delta\tau$ occur in the low trap concentration regime ($M < 1,500$), while for $M \rightarrow 3,000$, the difference diminishes sharply. This convergence of lifetimes with increasing trap density indicates a transition to a regime where the capture process is dominated by trap density rather than the geometric parameters of the pores.

To further quantify the variability in lifetime among small-radius pores (3a, 6a, 9a), we analyzed the range of τ values, defined as:

$$R_\tau(M) = \max(\tau_{3a}, \tau_{6a}, \tau_{9a}) - \min(\tau_{3a}, \tau_{6a}, \tau_{9a}), \quad (3)$$

Figure 5 presents the dependence of R_τ on M . The range R_τ provides a measure of the dispersion in lifetimes due to pore size differences, complementing the pairwise comparison in Fig. 4

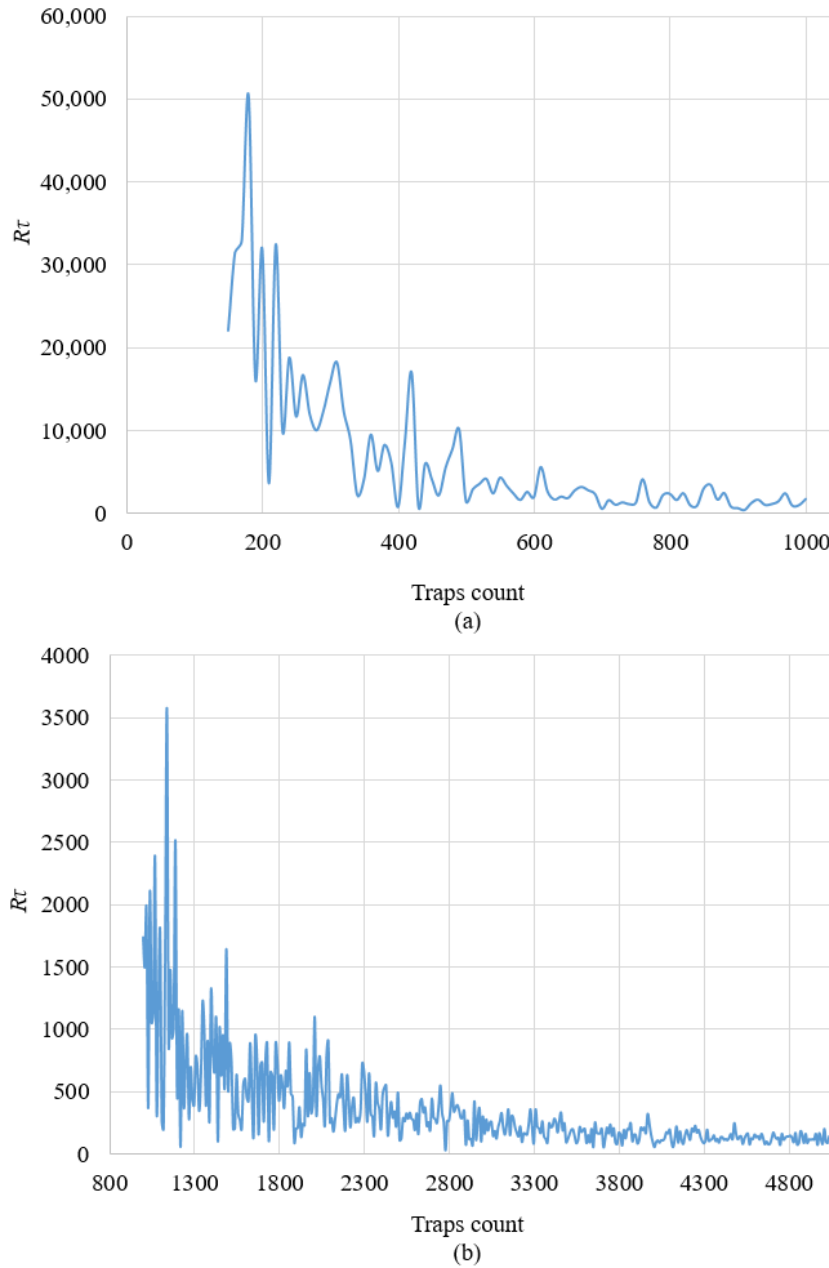


Figure 5. Lifetime range R_τ for small-radius pores as a function of trap concentration M . The top (a) corresponds to the low concentration regime ($M < 1,000$). The bottom (b) represents the high concentration regime ($M > 1,000$).

In the low trap concentration regime ($M < 1,000$), the range of lifetime values R_τ is significant, reaching up to 50,000 iterations. This indicates substantial variability in capture kinetics due to pore size effects at low trap densities. For $M > 1,000$, R_τ decreases monotonically with increasing M , reflecting the transition to a trap-density-dominated regime where geometric differences become less influential.

To further elucidate these observations, we analyze the pore size dependence of the maximum lifetime $\tau_{\max}$. Table 1 summarizes the pore radius at which the maximum lifetime $\tau_{\max}$ is achieved for each trap concentration M , providing insight into how optimal capture conditions shift with system parameters.

Table 1. Pore radius corresponding to the maximum lifetime $\tau_{\max}$ for varying trap concentrations M .

Pore radius	Number of configurations with maximum lifetime $\tau_{\max}$	%
3a	40	8,1
6a	56	11,3
9a	399	80,6

For trap concentrations exceeding $M > 2,000$, the maximum lifetime $\tau_{\max}$ was predominantly observed in pores of radius 9a, indicating that larger pores can sustain longer particle lifetimes under high trap density conditions. This result highlights the critical interplay between geometric confinement and trap density in determining capture kinetics. Specifically, while higher trap concentrations generally enhance capture efficiency, the pore radius modulates this effect by influencing diffusion paths and particle-surface interaction probabilities.

These findings underscore the necessity of simultaneously optimizing both geometric parameters (e.g., pore radius) and trap density when designing porous materials for applications requiring controlled particle capture or retention. Future work could extend this analysis to more complex pore geometries and broader parameter ranges to further refine design principles.

3.2. Approximation of Lifetime Dependence on Trap Concentration

As demonstrated in previous work [29], the lifetime τ , which characterizes the capture rate by traps, exhibits a strong dependence on trap concentration M . To quantitatively analyze this relationship, the range of M was divided into three distinct intervals based on concentration levels:

1. Low concentration: $M < 1,000$
2. Medium concentration: $1,000 < M < 2,000$
3. High concentration: $M > 2,000$

For each interval, three candidate functions were evaluated to approximate $\tau(M)$:

1. Hyperbola: $\tau(M) = a/M + b$
2. Quadratic hyperbola: $\tau(M) = a/M^2 + b$
3. Parabola: $\tau(M) = a + bM + cM^2$

Approximation was performed using nonlinear least-squares optimization via the *curve_fit* function from the *scipy* module in Python. The quality of each fit was assessed using the mean absolute error (MAE) between predicted and

simulated values. Detailed numerical results and error metrics are provided in Appendix C.

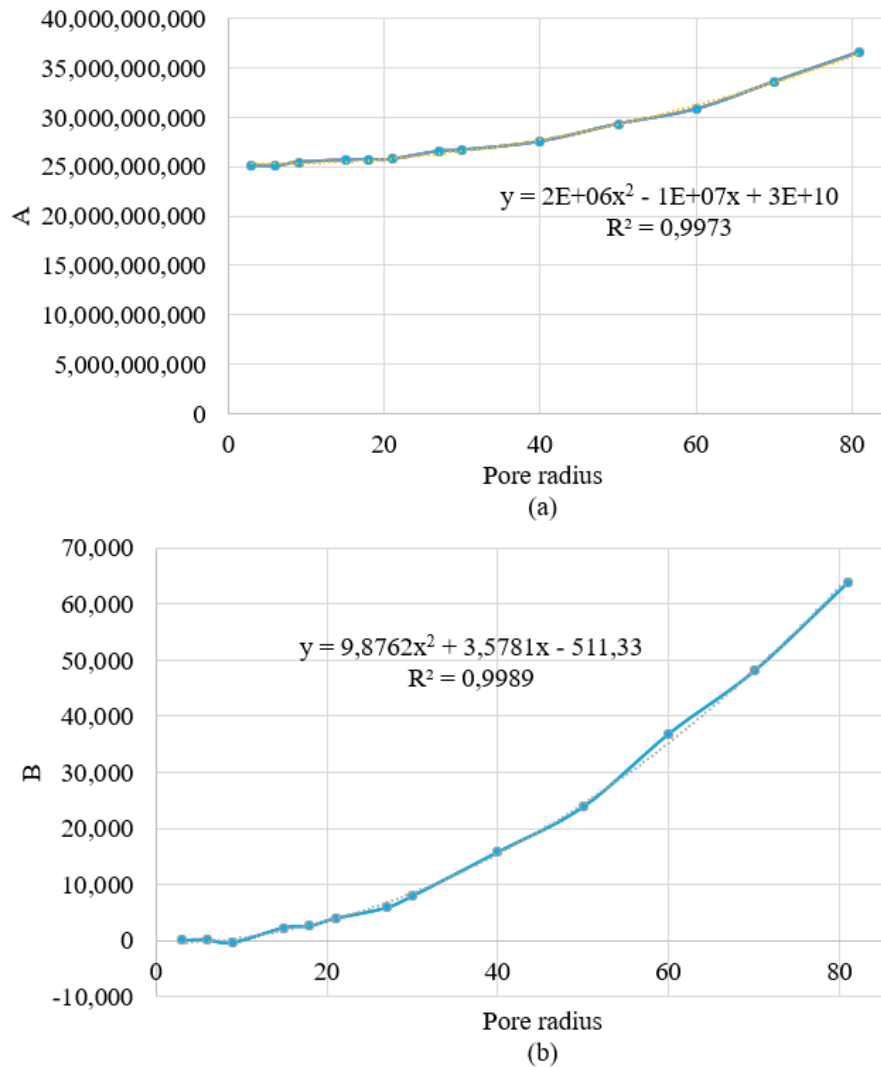
For all pore radii studied, the optimal approximating functions are established:

1. $M < 1000$: Quadratic hyperbola (captures initial steep decay)
2. $1000 < M < 2000$: Hyperbola (balances simplicity and accuracy)
3. $M > 2000$: Parabola (describes saturation behavior effectively)

The average approximation error for the selected functions was below 15% for all pores, meeting the acceptable accuracy threshold.

These results indicate a transition in the functional form of $\tau(M)$ across concentration regimes, reflecting underlying changes in the dominance of physical mechanisms, such as diffusion-limited capture at low M and transition to density-driven saturation at high M .

The dependence of the approximating function coefficients on pore radius was analyzed for both low and medium trap concentration regimes. Figure 6 illustrates the relationship between the coefficients A and B of the quadratic hyperbola $\tau(M) = A/M^2 + B$, used to model lifetime τ for $M < 1,000$, and the



pore radius R .

Figure 6. Dependence of approximation function coefficients on pore radius R for the low trap concentration regime ($M < 1,000$). The top (a) shows coefficient A of the quadratic hyperbola term, while panel (b) shows constant term B .

The nonlinear relationships demonstrate how geometric scaling affects capture kinetics parameters, with notable deviations observed for larger pore radii ($R > 60a$) due to finite-size effects and transition in diffusion regimes. A notable shift in the behavior of these coefficients is observed as the pore radius increases, with significant deviations occurring for larger radii (60a, 70a, 81a). These deviations can be attributed to the following factors:

1. Transition to a qualitatively distinct diffusion regime, where bulk diffusion characteristics become more dominant;
2. Manifestation of finite-size effects, as the pore dimensions approach the scale of the system;
3. Alterations in the nature of particle interactions due to reduced confinement.

The relationship between the coefficients and pore radius is nonlinear, particularly for coefficient B. A second-order polynomial approximation was applied to quantify this dependence:

For coefficient A: $A(R) = (175,637 R^2 - 604,571 R + 2,53 \times 10^6) \times 10^4$
with a coefficient of determination $R^2=0,9973$.

For coefficient B: $B(R) = 10,441 R^2 - 28,387 R - 311,530$
with $R^2=0,9989$.

The high R^2 values confirm the accuracy of the polynomial approximations, providing a reliable empirical basis for predicting coefficient behavior across varying pore radii.

Figure 7 illustrates the dependence of the coefficients A and B of the hyperbolic function $\tau(M) = A/M+B$ (used to approximate the lifetime τ for $1,000 < M < 2,000$) on the pore radius R.

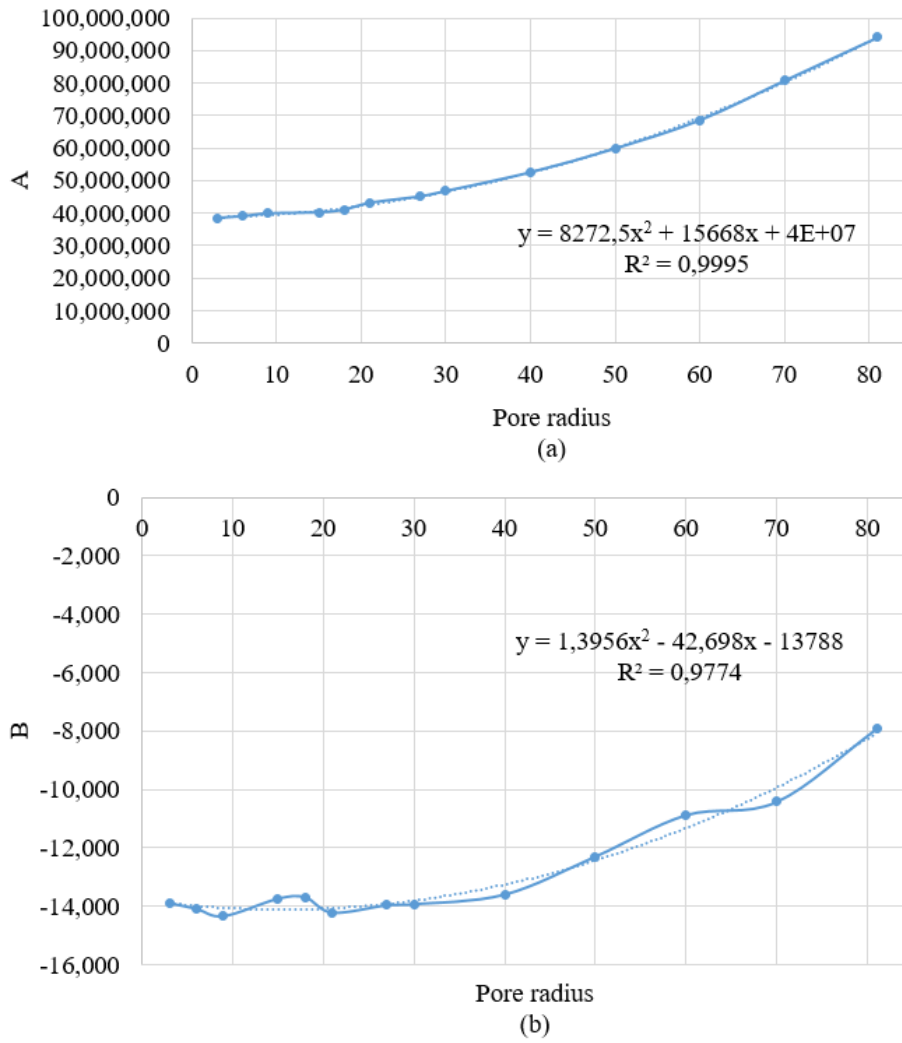


Figure 7. Dependence of approximation function coefficients on pore radius R for the low trap concentration regime ($1,000 < M < 2,000$). The top (a) shows coefficient A of the hyperbola term, while panel (b) shows constant term B .

The observed trends highlight the influence of pore size on capture kinetics in the medium concentration regime. To quantify this dependence, a second-order polynomial approximation was applied to both coefficients:

For coefficient A : $A(R) = (0,827 R^2 + 1,567 R + 3856,749) \times 10^4$

For coefficient B : $B(R) = 1,396 R^2 - 42,698 R - 13788,25$

The high-order polynomial model effectively captures the nonlinear relationship between the approximating function coefficients and the pore radius, underscoring the complex interplay between geometric confinement and trap distribution in the medium concentration regime. These empirical formulas serve as a predictive tool for estimating lifetime behavior across diverse pore sizes, highlighting the critical role of pore geometry in modulating capture efficiency.

The derived coefficients allow for the direct calculation of lifetime approximating functions, eliminating the need for further numerical simulations. To validate this approach, we assessed the performance of these functions against data for pore radii ranging from a to $81a$. A comparison of the approximation errors is presented in Table 2. The first row of the table

indicates the trap concentration range for which the lifetime was approximated, while the subsequent rows provide the following data:

- **SO**: The mean approximation error obtained from direct numerical fitting of the lifetime data.
- **SO₂**: The mean approximation error resulting from the application of the coefficient formulas derived above.

This comparison demonstrates the accuracy and utility of the empirical coefficient formulas in predicting lifetime behavior, reducing computational costs while maintaining high fidelity to the full numerical results.

Table 2. Comparison of approximation errors between direct fitting (SO) and formula-based (SO₂) methods.

		M < 1,000		1,000 < M < 2,000	
	R	SO	SO₂	SO	SO₂
a	3	13,	13,822	13,845	14,131
		854			
a	6	13,	13,485	13,478	13,612
		498			
a	9	13,	13,551	13,474	13,432
		462			
5a	1	-	13,38	12,697	12,595
8a	1	12,	12,283	11,757	11,589
		275			
1a	2	12,	12,776	10,762	10,456
		799			
7a	2	12,	12,12	10,322	10,302
		026			
0a	3	11,	11,335	10	9,937
		299			
0a	4	11,	11,1	8,216	8,373
		164			
0a	5	9,6	9,647	7,431	7,422
		17			
0a	6	10,	10,173	6,113	6,117
		427			
0a	7	9,6	9,721	5,494	5,527
		11			
1a	8	8,7	9,023	4,653	4,63
		68			

During the approximation procedure using the *curve_fit* function for the pore radius R=15a in the low concentration regime ($M < 1000$), a non-convergence error of the covariance matrix was encountered. However, application of the empirical coefficient formulas described in Section 3.2 yielded a satisfactory result, with a mean approximation error of 13,38.

In the low concentration range ($M < 1000$), the maximum discrepancy between the direct numerical approximation error (SO) and the formula-based error (SO₂) was 0,255 for R=81a, while the minimum discrepancy was 0,004 for R = 50a. The average discrepancy in this regime was 0,084. For the medium concentration range ($1,000 < M < 2,000$), the maximum discrepancy

reached 0,306 ($R = 21a$), the minimum was 0,015 ($R = 50a$), and the average discrepancy was 0,103.

Analysis of the accuracy of the two approximation methods (direct numerical fitting, SO, and the formula-based approach, SO₂) across different trap concentration ranges revealed the following key patterns:

1. **High Consistency:** Both methods exhibit exceptionally high consistency across all pore radii, with correlation coefficients $r > 0,998$ in both concentration ranges, confirming the reliability of the proposed empirical approach.

2. **Radius-Dependent Accuracy:** The mean approximation errors decrease systematically with increasing pore radius, reflecting the influence of geometric parameters on modeling accuracy.

3. **Small Discrepancies:** The maximum discrepancies between SO and SO₂ are 0,084 for $M < 1,000$ and 0,306 for $1,000 < M < 2,000$, representing less than 3% of the average error values in each regime.

4. **Statistical Validation:** The Wilcoxon signed-rank test confirmed the absence of statistically significant differences between the methods ($p > 0,38$), supporting the use of the formula-based approach for calculating approximating function coefficients.

These results demonstrate that the empirical coefficient formulas provide a computationally efficient and accurate alternative to direct numerical fitting, enabling reliable estimation of particle lifetimes without the need for extensive numerical experiments.

4. Discussion

Let us discuss the results obtained from the numerical simulation of particle diffusion in porous media. Our investigation reveals several key patterns regarding the influence of pore radius and trap concentration on the capture rate of diffusing particles:

1. **Behavior with Geometric Modulation:** The lifetime (τ) of particles exhibits a similar dependence on the number of traps (M) across various pore radii. However, for significantly larger radii ($R > 50a$), this dependence undergoes substantial modifications. These changes are attributed to a transition into a qualitatively different diffusion regime, where finite-size effects and diminished confinement alter particle dynamics.

2. **Concentration-Driven Convergence:** The difference in lifetime values for different pore radii markedly decreases as trap concentration increases. This convergence indicates that at high trap densities, the capture process becomes dominated by the abundance of traps rather than by geometric constraints.

3. **Identification of Capture Regimes:** Three distinct operational regimes for particle capture were identified and characterized based on trap concentration:

- **Low concentration regime** ($M < 1,000$): Capture is strongly influenced by diffusion limitations and pore geometry.

- **Medium concentration regime** ($1,000 < M < 2,000$): A transition region where both trap density and geometry play significant roles.

- **High concentration regime** ($M > 2,000$): Capture is primarily controlled by trap density, with geometric parameters having a diminished effect.

4. Optimal Approximation Functions: For each regime, an optimal approximating function was determined:

- Low concentrations ($M < 1,000$): $\tau(M) = b + a/M^2$
- Medium concentrations ($1,000 < M < 2,000$): $\tau(M) = b + a/M$
- High concentrations ($M > 2,000$): $\tau(M) = a + bM + cM^2$

5. Empirical Coefficient Calculation: We proposed a method for calculating the coefficients of these approximating functions using empirical relationships derived from the pore radius. A comparative evaluation with directly fitted functions demonstrates the high accuracy of this method, providing a reliable and computationally efficient predictive tool.

The findings of this study are significant for the design and engineering of porous materials with tailored sorption properties. The developed approximation dependencies enable the prediction of particle capture kinetics across a wide range of geometric parameters, facilitating the optimization of material performance for specific applications.

The investigation of diffusion processes and capture by traps is also important for cell metabolism and protein activity [34]. The processes of water transfer are responsible for the diffusion of nutrients, metabolic exchange, and ion transport within bone structures. They contribute to the mechanism of bone adaptation, the stabilization of the mineral structure, and the interaction between minerals and collagen [35-37].

Author Contributions:

Conceptualization, V.A., B.K.; methodology, V.A., B.K.; software, B.K., D.D.; validation, B.K., S.M.; formal analysis, V.A., B.K.; investigation, V.A.; resources, B.K., S.M.; data curation, S.M.; writing—original draft preparation, V.A., B.K.; writing—review and editing, V.A., B.K.; visualization, S.M., D.D.; supervision, V.A.; project administration, V.A.; funding acquisition, V.A. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement:

The original materials presented in this study are hosted on the github repository: https://github.com/bairinc0/MDPI_Diffusion_3_D_pores_comprasion (03 October 2025). Further inquiries can be directed to the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

Appendix A

Algorithm of Simulations for Diffusion Processes in Media with Traps

Let us briefly describe the modeling algorithm in cylindrical pores with traps on the surfaces of cylinders. Particles undergo random walk diffusion within a cylindrical pore. We modeled particle movement as a discrete step of size $1a$ in one of the coordinate directions. At each iteration, a random number generator selects the direction of movement (i.e., the coordinate to change). We evaluate the following boundary and interaction conditions:

1. Free Position Movement: If the target coordinate is unoccupied, the particle moves to the new position.

2. Obstacle Encounter: If the target coordinate is occupied, the particle remains at its current position.

3. Boundary Condition: Upon reaching the cylindrical boundary without trap, the particle returns to its previous position.

4. Trap Interaction: If a particle attempts to move to a lattice site occupied by a trap, the particle is permanently captured and removed from the simulation, and the trap is simultaneously deactivated.

All numerical simulations were implemented in C++ (ISO C++17 standard) using the Visual Studio 2022 development environment. To ensure statistical reliability and robustness of the results, we perform 20 independent runs for each unique parameter set. We used the Mersenne Twister algorithm (mt19937) to generate random numbers.

Placing of traps

This study presents a comparative analysis of particle capture efficiency in cylindrical pores with different radii, under constant trap concentration conditions. The simulations established that the use of identical spatial distributions of traps relative to the cylindrical coordinate system (i.e., same axial z and angular θ positions) for different pore radii is essential for ensuring a valid and controlled comparison of capture kinetics. This approach isolates the effect of pore geometry by eliminating confounding variables associated with random variations in trap placement. Trap positions were defined in a cylindrical coordinate system as $(R_n \cos \theta, R_n \sin \theta, z)$, where R_n is the pore radius, θ is the azimuthal angle, and z is the axial coordinate. We used the following algorithm to generate trap placements:

1. Coordinate Sampling: The axial coordinate z and the azimuthal angle θ were independently sampled from uniform distributions over predefined intervals $[z_{\min}, z_{\max}]$ and $[0, 2\pi)$, respectively.

2. Radial Coordinate: The radial coordinate was fixed to the pore radius R , where $R \in \{3a, 6a, 9a, 15a, 18a, 21a, 27a, 30a, 40a, 50a, 60a, 70a, 81a\}$.

3. Discretization: The calculated Cartesian coordinates (x, y, z) were discretized by truncating the fractional part, mapping them to the simulation lattice.

This approach ensures that the relative distribution of traps along the axial and angular coordinates is identical for all pore radii, isolating the effect of the radius change itself. Maintaining this consistency in trap placement along z and θ is essential for the rigorous comparison of capture dynamics across varying pore sizes, as it isolates the effect of radius change from random variations in trap layout.

Appendix B

Lifetime Achievement Analysis

Using the developed algorithm, we generated 500 distinct spatial configurations of traps. The trap concentration M varied across the range $100 \leq M \leq 5,090$ with a discrete step size of $\Delta M = 10$. For each value of M , identical spatial distributions of traps were created for the entire set of studied pore radii: $\{3a, 6a, 9a, 15a, 18a, 21a, 27a, 30a, 40a, 50a, 60a, 70a, 81a\}$.

Computational Parameters:

- Number of independent simulation runs per configuration: 20
- Initial number of particles, N_0 : 200

- Maximum number of iterations per simulation: 1,000,000

The minimum concentration of traps required to determine the lifetime meaningfully is $M > 125$. This threshold is derived from the definition of lifetime, where $N_t = N_0/e \approx 74$, ensuring a sufficient number of capture events for statistical significance. At these low concentrations, nearly all traps participate in the capture process. The corresponding lifetime statistics for this low-concentration regime are presented in Table B1.

Table B1. Calculated particle lifetime (τ) statistics for the low trap concentration regime ($M > 125$).

M/R	3a	6a	9a	15a	18a	21a	27a	30a	40a	50a	60a	70	81a
	a												
130	0	0	0	0	0	0	0	0	0	0	0	0	0
140	0	0	0	0	0	0	0	0	0	0	0	0	0
150	18	18	18	13	16	16	11	10	10	3	0	0	0
160	3	6	1	4	1	3	3	1	2	0	0	0	0
170	20	20	19	19	20	19	18	20	15	10	9	2	0
190	20	20	20	20	20	20	20	20	20	20	16	11	7
200	20	20	19	20	19	20	20	20	20	15	16	12	7
210	20	20	20	20	20	20	20	20	20	20	20	18	19
220	20	20	20	20	20	20	20	20	20	20	20	20	20

A value of '0' indicates that the lifetime τ could not be reliably determined (insufficient capture events) for the given M and R.

The table is structured with the pore radii listed in the header and the number of traps M in the first column. Analysis of the results reveals the following key findings:

The lifetime behavior stabilizes (i.e., is consistently achieved across all simulation runs) for pore radii in the range 3a to 60a when the number of traps meets or exceeds $M \geq 210$.

For larger pore radii (70a and 81a), a similar stabilization of lifetime behavior occurs at a slightly higher trap count of $M \geq 220$.

This observed difference in the stabilization threshold highlights the influence of pore geometry on the capture process. The increased volume and surface area of larger pores require a higher density of traps to achieve a consistent and reliable measurement of the particle lifetime, as the characteristic diffusion time scales with the system size.

Appendix C

Approximation

A visual analysis of the obtained dependencies $\tau(M)$ was conducted, leading to the evaluation of three distinct approximating functions for each concentration interval:

1. Hyperbola: $\tau(M) = a/M + b$

2. Quadratic hyperbola: $\tau(M) = a/M^2 + b$

3. Parabola: $\tau(M) = a + bM + cM^2$

The quality of each approximation was quantified using the mean absolute error (MAE) between the model predictions and the simulation data. The results of this analysis, including the MAE for each function and pore radius, are summarized in Table C1.

Table C1. Mean absolute error (MAE) of the approximating functions for the lifetime $\tau(M)$ across different pore radii.

	Low concentration		Medium concentration		High concentration
R	MAE		MAE		MAE
	(Hyperbola)	(Quadratic Hyperbola)	(Hyperbola)	(Quadratic Hyperbola)	
					(Parabola)
3a	29,93	13,854	13,845	46,197	13,877
6a	30,18	13,498	13,478	45,355	14,215
9a	30,751	13,462	13,474	44,691	13,294
15a	28,387	120,041	12,697	12,469	11,659
18a	27,965	12,275	11,757	11,509	10,555
21a	28,027	12,799	10,762	10,555	9,974
27a	26,088	12,026	10,322	36,932	7,943
81a	12,168	8,768	4,653	20,722	3,147

The table presents the values of the mean absolute error (MAE) for the approximating functions across different pore radii. The first row specifies the trap concentration ranges (M). The second row contains the headers for the approximating functions: hyperbola ($\tau(M) = a/M+b$), quadratic hyperbola ($\tau(M) = a/M^2+b$), and parabola ($\tau(M)=a+bM+cM^2$). The first column lists the pore radii, while the main body of the table displays the corresponding MAE values.

Hyperbolic functions were applied for low and medium concentration regimes; however, for high concentrations ($M > 2,000$), these functions did not yield acceptable accuracy. Following established recommendations, where the mean approximation error should not exceed 15%, our results support the use of the following functions for each concentration regime:

1. **Low concentration** ($M < 1,000$): Quadratic hyperbola ($\tau(M) = a/M^2+b$)
2. **Medium concentration** ($1,000 < M < 2,000$): Hyperbola ($\tau(M) = a/M+b$)
3. **High concentration** ($M > 2,000$): Parabola ($\tau(M) = a+bM+cM^2$)

This selection ensures optimal accuracy and reliability in predicting particle lifetime across diverse geometric and trap concentration conditions.

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